

# Variational Wave Function for Generalized Wigner Lattices in One Dimension

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## Abstract

We study a system of electrons on a one-dimensional lattice, interacting through the long range Coulomb forces, by means of a variational technique which is the strong coupling analog of the Gutzwiller approach. The problem is thus the quantum version of Hubbard's classical model of the generalized Wigner crystal [J. Hubbard, Phys. Rev. B **17**, 494 (1978)]. The magnetic exchange energy arising from quantum fluctuations is calculated, and turns out to be smaller than the energy scale governing charge degrees of freedom. This approach could be relevant in insulating quasi-one-dimensional compounds where the long range Coulomb interactions are not screened. In these compounds charge order often appears at high temperatures and coexists with magnetic order at low temperatures.

## 1 INTRODUCTION

The Luttinger Liquid is a paradigm for models of one-dimensional interacting electrons. Remarkably, it not only holds for weak (bare) couplings, but remains valid up to strong couplings (for the special case of the Hubbard model up to  $U = \infty$ ). For short-range interactions, a small set of coupling constants, corresponding to forward, backward and Umklapp scattering, determines the low-energy behavior. For long-range interactions, such as the unscreened Coulomb interaction, the dependence of the forward scattering on momentum transfer  $q$  has to be taken into account, as this term diverges logarithmically for  $q \rightarrow 0$ . Nevertheless, the method of bosonization, which is so useful for weak short-range couplings, can be extended to this case. As shown by Schulz, this method predicts a ground state with quasi-long-range charge order for the homogeneous electron gas with long-range ( $1/r$ ) Coulomb interaction [2]. This behavior is found to hold up to the limit of a very dilute gas where the Coulomb interaction dominates and the ground state is a (Wigner) crystal of electrons with strongly localized wave functions.

For narrow-band materials the effects of the underlying lattice have to be taken into account. For the case of Coulomb interactions this has been pointed out by Hubbard [1], who considered the extreme limit of zero bandwidth. In this case the problem is equivalent to that of a system of classical

charges distributed over the sites of a lattice and coupled to each other by the Coulomb interaction. We have extended Hubbard's considerations to a more realistic model including a small but finite hopping term. Using a variational wave function we are not only able to describe the incipient charge delocalization, but also to account for an antiferromagnetic interaction induced by the exchange of electrons located on the neighboring sites of the Wigner lattice [3]. For a small hopping amplitude  $t$  the energy scale for the charge degrees of freedom turns out to be much larger than that for the spin degrees of freedom.

## 2 VARIATIONAL APPROACH

We consider a system of one-dimensional fermions interacting via a local repulsion  $U$  and a long-range Coulomb potential  $V_m = V/|m|$ . The corresponding tight-binding Hamiltonian is

$$H = -t \sum_{i\sigma} (c_{i,\sigma}^+ c_{i+1,\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i \neq j} V_{i-j} n_i n_j, \quad (1)$$

where  $n_i = n_{i\uparrow} + n_{i\downarrow}$  measures the density per site. The Fourier transform of the Coulomb potential is  $V(q) \sim -2V \log q$  for  $q \rightarrow 0$  (we set the lattice constant equal to 1). In the following we limit ourselves to the case of a quarter-filled band (i.e., an average electron density of  $n = 1/2$  per site). Hubbard's classical solution is then an alternation of occupied and empty sites, corresponding to a  $4k_F$  charge modulation and uncoupled spin degrees of freedom.

For finite but small  $t$  we use the variational ansatz

$$|\Psi_B\rangle = e^{-\eta \hat{T}} |\Psi_\infty\rangle, \quad (2)$$

where  $\eta$  is a variational parameter,  $\hat{T}$  is the kinetic energy operator and  $|\Psi_\infty\rangle$  is the ground state for  $t = 0$ , i.e., Hubbard's classical solution. This wave function, introduced as a counterpart of the Gutzwiller ansatz to describe the ground state of the large  $U$  Hubbard model at half filling [4], has been successfully applied to the Mott-Hubbard transition [5]. The role of the operator  $e^{-\eta \hat{T}}$  is analogous to that of  $e^{-\lambda \hat{D}}$  in Gutzwiller's wavefunction, where double occupancy is suppressed in order to reduce the weight of configurations with high potential energy. Here the factor  $e^{-\eta \hat{T}}$  suppresses states with high kinetic energy. In the limit  $\eta \rightarrow \infty$  only the state with the lowest kinetic energy, i.e., the Fermi sea, survives.

For very large  $U$ , where double occupancy is expected to be completely suppressed, the charge degrees of freedom can be described in terms of spinless fermions coupled by long-range Coulomb forces, whereas the spin degrees of freedom are uncoupled. For spinless fermions, the variational energy is readily calculated and turns out to be very close to the Hartree-Fock approximation [3]. The relevant scale for charge excitations is the energy required for moving an electron from its position in the classical Hubbard configuration to an empty neighboring site, i.e.

$$\Delta_c = V \sum_{l=1}^{\infty} \frac{1}{l[(2l)^2 - 1]} \approx 0.39V. \quad (3)$$

Note that the charge gap would be larger ( $\Delta_{nn} = 0.5V$ ) if we only retained interactions between electrons on nearest neighbors. This simple argument shows that even though the ground state configuration is well described by an "extended" Hubbard model, the spectrum of excited states is different when the long-range tail of the Coulomb potential is taken into account. In the latter case, the system is "softer" with respect to charge fluctuations.

For finite but large values of  $U$ , the double occupancy does not vanish but is expected to be small. In order to take this effect into account we consider a refined wave function

$$|\Psi_{BG}\rangle = e^{-\lambda\hat{D}}e^{-\eta\hat{T}}|\Psi_{\infty}\rangle, \quad (4)$$

where  $\hat{D}$  measures the number of doubly occupied sites. The starting ground state  $|\Psi_{\infty}\rangle$  is now a superposition of all possible configurations of spins attached to the even (or odd) sites of the chain. The operator  $e^{-\eta\hat{T}}$  again controls the delocalization of electrons away from their classical site, while the Gutzwiller operator  $e^{-\lambda\hat{D}}$  reduces the weight of configurations with doubly occupied sites. The ansatz (4), introduced for the Hubbard model by Otsuka [6], leads to a dramatic improvement of the ground state energy, as demonstrated for the exactly soluble one-dimensional Hubbard model with long-range hopping [7]. For small  $t$ , the energy can be worked out as an expansion in  $t/V$ , in close analogy to the procedure used for the Hubbard model [4]. In the large  $U$  limit we obtain for the minimum of the variational energy per site [3]

$$\epsilon_{BG} = -\frac{1}{2\log 2 - 1} \frac{t^2}{V} + J \langle \Psi_{\infty} | \sum_i ' \left( \mathbf{S}_i \mathbf{S}_{i+2} - \frac{1}{4} n_i n_{i+2} \right) | \Psi_{\infty} \rangle, \quad (5)$$

where the sum runs over all even sites and the exchange constant is given by

$$J = \frac{36 \log 2 \, t^4}{(15 - 16 \log 2)(2 \log 2 - 1)^2 V^3 + 6(2 \log 2 - 1)^2 V^2 U}. \quad (6)$$

The first term in Eq. (5) is identical to the variational energy for spinless electrons in the large  $V$  limit (or the spinful case for  $U \rightarrow \infty$ ). Here we see that for finite  $U$  we obtain an antiferromagnetic coupling between the spins. The remaining problem of finding the best magnetic state is equivalent to the problem of determining the ground state of the one-dimensional Heisenberg model. Its solution is known thanks to Bethe. Recently it has been shown that the spin correlations decay like  $(-1)^{(i-j)}(\log|i-j|)^{\frac{1}{2}}/|i-j|$  [8]. Therefore our variational wave function exhibits long-range charge order and algebraic magnetic order.

### 3 DISCUSSION

In this work, we have studied a one-dimensional system of electrons interacting through the long-range Coulomb forces. Starting from the strong coupling generalized Wigner lattice, we have introduced a variational wave function which allows to treat the effects of quantum fluctuations. As a result, magnetic correlations develop out of the charge ordered configuration, with a lower energy scale.

Quasi one-dimensional organic compounds of the  $(\text{TMTTF})_2\text{X}$  family [9], as well as the inorganic materials  $(\text{DI-DCNQI})_2\text{X}$  [10], are known to exhibit charge ordered structures at temperatures  $T \sim 100 - 200\text{K}$ . There are several experimental indications that the long-range electron-electron interactions are the common driving mechanism of the charge ordering: (i) the measured electronic conductivities are low, suggesting that the long-range tail of the Coulomb potential is not screened; (ii) a strong  $4k_F$  superstructure, inferred from both X-ray and NMR spectroscopy, develops in the charge ordered region, which can not be ascribed to an ordinary  $2k_F$  Fermi surface instability; (iii) the  $4k_F$  ordering is not necessarily associated to a structural transition; (iv) charge ordering sets in at a much higher temperature than magnetic ordering.

In such compounds, where the filling is fixed by stoichiometry to one carrier every two sites, electron-electron correlations are generally treated theoretically in the framework of the extended

Hubbard model, which only retains on-site and nearest-neighbors interactions [11]. Although this can successfully reproduce the  $4k_F$  charge correlations, new physics can in principle be expected if the full long-range potential is taken into account. For example, in the metallic regime, it is known that quasi-long-range order appears in purely one-dimensional systems due to the strong forward scattering associated to the  $1/r$  behavior at long distances, regardless of the interaction strength [2]. In the charge ordered regime, which is the object of the present work, the spectrum of excited states can differ substantially from what expected in the extended Hubbard model. The charge gap is lower, leading to stronger charge fluctuations, and to larger magnetic exchange energies. In compounds where the filling differs from  $n = 1/2$ , such as the TTF TCNQ (studied by Hubbard [1]), the use of the extended Hubbard model is even more debatable.

Clearly, the phenomenology observed in quasi-one-dimensional compounds is much more complex than what emerges from the simple model considered here. The detailed phase diagrams are determined by the chain dimerization, anion size and symmetry, inter-chain couplings, etc. However, the ubiquitous experimental signatures of the electron-electron interactions in such insulating systems call for a more systematic study of the role of the long-range Coulomb interactions.

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